

Methyl acetate
79-20-9 | DTXSID4021767

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 60.3 °C

Global applicability domain: Inside

Local applicability domain index: 7.44e-01

Confidence level: 8.51e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methyl acetate</div> <div>Measured: 56.8</div> <div>Predicted: 60.3</div>	<div>Image not found</div> <div>Ethyl formate</div> <div>Measured: 54.4</div> <div>Predicted: 60.0</div>	<div>Image not found</div> <div>2-Methylpropanal</div> <div>Measured: 64.5</div> <div>Predicted: 67.6</div>
<div>Image not found</div> <div>Methyl ethyl ketone</div> <div>Measured: 79.5</div> <div>Predicted: 72.4</div>	<div>Image not found</div> <div>Butyraldehyde</div> <div>Measured: 74.8</div> <div>Predicted: 71.3</div>	